
































# Exhibit B




































W0299




































**Automated Molecular Replacement.** Charles R. Kissinger and Bradley A. Smith, Pfizer, Inc. 11099 North Torrey Pines Rd., La Jolla, CA 92037.

New molecular replacement (MR) techniques have made it feasible to screen large databases of protein structures or structural fragments to extract the best available search model for a particular MR problem. The use of stochastic search techniques, such as simulated annealing or evolutionary algorithms, to carry out rapid six-dimensional (or higher) MR searches has proven to be a robust method for solving MR problems. This approach can be extended to make large-scale, highly automated search-model screening practical. We have developed a program, EPMR, which performs automated six-dimensional MR searches using an evolutionary optimization algorithm. We have examined the limits of effectiveness of this method with regard to search model quality, data quality, and alternative scoring criteria, and we are now exploring a variety of methods for extending this approach to make use of large structural databases. A highly parallel version of EPMR for multi-processor machines and computing clusters has been developed which allows multiple search models to be evaluated simultaneously. The evolutionary search procedure also has been extended to include selection of the optimal member of a set of search models during the course of the evolutionary search. We are now exploring the practicality of searching simultaneously with smaller structural fragments to allow the molecular model to be constructed during the search. The limits of these procedures with respect to database size and search model quality will be discussed.

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


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


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

















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





























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


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	<a href="#">W0153.html</a>	30-Mar-2001 12:02	3k
	<a href="#">W0154.html</a>	30-Mar-2001 12:02	3k
	<a href="#">W0155.html</a>	30-Mar-2001 12:02	2k
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	<a href="#">W0157.html</a>	30-Mar-2001 12:02	2k
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	<a href="#">W0159.html</a>	30-Mar-2001 12:02	2k
	<a href="#">W0160.html</a>	30-Mar-2001 12:03	3k
	<a href="#">W0161.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0162.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0163.html</a>	30-Mar-2001 12:03	3k
	<a href="#">W0164.html</a>	30-Mar-2001 12:03	3k
	<a href="#">W0165.html</a>	30-Mar-2001 12:03	3k
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	<a href="#">W0167.html</a>	30-Mar-2001 12:03	3k
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



















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






















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	<a href="#">W0173.html</a>	30-Mar-2001 12:03	2k
	<a href="#">W017300.gif</a>	30-Mar-2001 09:32	1k
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	<a href="#">W0177.html</a>	30-Mar-2001 12:03	3k
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	<a href="#">W0203.html</a>	02-Apr-2001 14:16	2k

	<a href="#">W0204.html</a>	02-Apr-2001 14:16	3k
	<a href="#">W0205.html</a>	02-Apr-2001 14:16	3k
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	<a href="#">W0210.html</a>	04-Apr-2001 18:26	2k
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	<a href="#">W0212.html</a>	02-Apr-2001 14:16	3k
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	<a href="#">W0216.html</a>	04-Apr-2001 18:26	3k
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	<a href="#">W0218.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W021800.gif</a>	04-Apr-2001 15:24	259k
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	<a href="#">W0221.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0222.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0223.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0224.html</a>	04-Apr-2001 18:26	2k
	<a href="#">W0225.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0226.html</a>	04-Apr-2001 18:26	4k
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	<a href="#">W0228.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0229.html</a>	04-Apr-2001 18:26	4k
	<a href="#">W0230.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W023000.gif</a>	12-Apr-2001 07:55	450k
	<a href="#">W0231.html</a>	04-Apr-2001 18:26	6k
	<a href="#">W0232.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0233.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0234.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0235.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0236.html</a>	04-Apr-2001 18:26	2k

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














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

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	<a href="#">W0240.html</a>	04-Apr-2001 18:26	2k
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	<a href="#">W0242.html</a>	04-Apr-2001 18:26	3k
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	<a href="#">W0245.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0246.html</a>	04-Apr-2001 18:26	2k
	<a href="#">W0247.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0248.html</a>	04-Apr-2001 18:26	4k
	<a href="#">W0249.html</a>	04-Apr-2001 18:26	2k
	<a href="#">W0250.html</a>	04-Apr-2001 18:26	3k
	<a href="#">W0251.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0252.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0253.html</a>	12-Apr-2001 11:54	2k
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	<a href="#">W0256.html</a>	27-Apr-2001 13:39	2k
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	<a href="#">W0258.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0262.html</a>	12-Apr-2001 11:54	3k

	<a href="#">W0263.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0264.html</a>	12-Apr-2001 11:54	4k
	<a href="#">W0265.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0266.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0267.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0269.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0270.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0271.html</a>	12-Apr-2001 11:54	4k
	<a href="#">W0272.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0273.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0274.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0275.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0276.html</a>	12-Apr-2001 11:54	5k
	<a href="#">W0277.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0278.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0279.html</a>	12-Apr-2001 11:54	2k
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	<a href="#">W0282.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0285.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0287.html</a>	12-Apr-2001 11:54	4k
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	<a href="#">W029400.gif</a>	12-Apr-2001 07:55	2k
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


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	<a href="#">W0297.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0298.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0299.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0300.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0301.html</a>	12-Apr-2001 11:54	2k
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	<a href="#">W0304.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0305.html</a>	12-Apr-2001 11:54	4k
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	<a href="#">W0307.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0309.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0310.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0311.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0316.html</a>	12-Apr-2001 11:54	2k
	<a href="#">W0317.html</a>	12-Apr-2001 11:54	4k
	<a href="#">W0318.html</a>	18-Apr-2001 14:15	3k
	<a href="#">W0319.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0320.html</a>	12-Apr-2001 11:54	4k
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	<a href="#">W0323.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0329.html</a>	12-Apr-2001 11:54	4k

	<a href="#">W0330.html</a>	12-Apr-2001 11:54	4k
	<a href="#">W0331.html</a>	12-Apr-2001 11:54	4k
	<a href="#">W0332.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W033200.gif</a>	12-Apr-2001 07:55	3k
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	<a href="#">W033300.gif</a>	12-Apr-2001 07:55	2k
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	<a href="#">W0337.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W033701.gif</a>	12-Apr-2001 11:40	1k
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	<a href="#">W0339.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0340.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0343.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0344.html</a>	23-Apr-2001 11:43	1k
	<a href="#">W0345.html</a>	23-Apr-2001 11:43	3k
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	<a href="#">W0348.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0349.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0350.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0351.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0352.html</a>	12-Apr-2001 11:54	2k
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	<a href="#">W0354.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0355.html</a>	12-Apr-2001 11:54	3k

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


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	<a href="#">W035801.gif</a>	12-Apr-2001 15:24	1k
	<a href="#">W0359.html</a>	12-Apr-2001 11:54	2k
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	<a href="#">W0363.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0364.html</a>	12-Apr-2001 11:54	3k
	<a href="#">W0365.html</a>	23-Apr-2001 11:43	4k
	<a href="#">W0366.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0368.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0369.html</a>	12-Apr-2001 11:54	3k
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	<a href="#">W0371.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0372.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0373.html</a>	23-Apr-2001 11:43	3k
	<a href="#">W0374.html</a>	18-Apr-2001 14:15	2k
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